# Ion accelerator based radiation simulations of neutron damage in reactors: issues and challenges in experiments and modeling

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**Abstract:** Using accelerator-based ion bombardment as a surrogate irradiation source to simulate neutron damage in reactors is important to understand and predict materials degradation under extreme conditions. Challenges and issues, however, exist in both experimental and modeling studies. Major issues being discussed include (1) how to identity and understand neutron-atypical artifacts introduced in accelerator-based ion irradiations. Examples on defect imbalance and pulse beam effects are given; (2) how to standardize experimental procedures for ion irradiation testing. Examples on accelerator setups and beam control are given; (3) how to develop modeling capabilities to understand structural changes. Examples of Monte Carlo simulations, Kinetic Monte Carlo simulations and molecular dynamics simulations are given. Several methods to alleviate the issues are further discussed.

**Keyword:** radiation damage; accelerator; simulation;

## 1 Introduction[1]

Nuclear reactors represent extremely harsh environments combining high pressure, corrosion, high temperature and high damage levels [1]. Particularly, when accompanied with neutron irradiation damage, many unique materials degradation phenomena occur, which cannot be described by traditional mechanical property and structural changes under normal irradiation-free harsh conditions. Examples include irradiation-induced stress corrosion cracking which occurs only when stress, corrosion, and neutron damage present together [2]. Another example is high temperature creep. Although permanent dimension changes due to creep is well known in high temperature applications in aerospace engineering, creep failures are accelerated when neutron damage is introduced [3]. Overall, materials issues inside reactors cannot be separated from neutron damage, which come up unique challenges in nuclear materials studies.

The most straightforward materials testing in nuclear engineering is using research reactors. However, there are two issues: one is that the amount of time required to achieve damage levels expected from designs is unrealistically long. For example, Advanced Testing Reactor (ATR) at Idaho National Laboratory is able to achieve about 10 dpa or less per year, and the BOR-60 research reactor in Russia is able to achieve about 20 dpa per year. For Generation IV reactors, in core components expect to have damage levels beyond 200 displacements per atom (dpa) [4], which means reactor-based materials testing will require decades to finish one experiment. The other issue for reactor testing is the amount of radioactivity after reactor irradiation. For most university research laboratories, characterization often uses public user facilities which have limits on sample radioactivity.

As a surrogate irradiation source, ion accelerators have been widely used to simulate neutron damage [5]. Ion accelerators use energetic atoms to create damage. The largest benefit of accelerator testing is that damage rates are typically a few orders of magnitude higher that of neutrons. Therefore, much faster materials screening and testing can be realized. The amount of radioactivity after ion irradiation is very limited and generally ignorable (except for high energy ion irradiation by lights ions such as hydrogen).

However, it has been a long debate whether ion accelerator testing can have a one-to-one correlation established with reactor testing. Major concerns include: first, ion irradiation only damages a near surface region about a few microns deep. The microstructure changes and defect evolution could be very different from reactor radiation, particularly when grain sizes of materials are larger than ion

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damage depth. Grain boundaries act as defect sinks [6], and whether they participate in defect processing plays a role to determine final structural changes.

Second, ion irradiation may not develop "correct" phases as expected in reactor irradiation. Early studies in the US Liquid Metal Reactor program in 1980s have shown that accelerated ion irradiation was unable to develop the exact phase evolution characteristic of long-term neutron irradiation that usually preceded the onset of void swelling [7]. This is a big issue for swelling-resistant alloys where such phase evolution is critical to end incubation period of swelling.

Third, ion irradiation is performed with dpa rates a few orders of magnitude higher than a typical reactor testing. The rate of dpa creation may become a key parameter, in additional to dpa, to influence microstructural changes. "Temperature shifting" has been proposed to consider dpa rate effects and obtain equivalence of accelerator testing to reactor testing [8], but it has been a debate whether such shifting truly exists.

Forth, shallow damage depths also impose a great challenge on mechanical property testing. Although various tools such as nanoindentation have been developed to characterize mechanical properties of near surface regions, there is a gap between results extracted from micron size testing and true mechanical behaviors of bulk materials used in reactors [9].

In parallel, understanding radiation effects through modeling is also greatly challenged. Various modeling approaches have been developed but the successes are limited to their unique length and time scales. How to link quantum mechanics to continuum methods to obtain capabilities of multiscale modeling at the mescoscale still has a long way to go [10][11]. The benefits of multiscale modeling are two folds: an experimental validated modeling is able to predict materials behaviors beyond the experimentally achievable conditions and is able to provide insights and feedbacks required for materials development.

Above shortcomings or issues have been well known and well documented in literature. Below, we review some new issues observed recently which require attentions for both experimental and modeling studies.

# 2 Issues in experimental studies

## 2.1 Dose determination

It has been a general consensus that dpa can be used as a normalization parameter to bridge ion accelerator and neutron irradiation [1]. However, it has been recently recognized that the dpa levels quoted in most published US and European ion studies have been overestimated by a factor of ~2 by choosing the wrong option in the SRIM code (Full Cascade vs. correct Kinchin-Pease) [12], thereby now requiring twice as long to reach any given neutron-equivalent dose level for those facilities that were using the Full Cascade method to calculate dpa.

## 2.2 Defect imbalance

For almost all ion irradiation experiments so far, it was found that void swelling is peaked at a depth corresponding to half of the projected range of implants. This is unexpected if dpa is only parameter determining swelling. Since nuclear stopping power is peaked at a few keVs for most metal implants, the dpa curve is slightly shallower but very close to profile of implants. Figure 1 is statistical analysis of void swelling caused by 3.5 MeV Fe self ions in Fe at irradiation temperature of 450 ℃. With increasing Fe ion doses, void swelling increases at a depth of about 200 nm to 800 nm, which deviates from the dpa profile calculated by using SRIM code. This can be explained by the following [13]: since ion irradiation transfers momentum in the forward direction, distributions of interstitials and vacancies are slightly different. Interstitials are positioned deeper than that of vacancies. Assuming a perfect defect recombination in interstitial-vacancy overlapping region, calculation of defect imbalance, the defect number difference between local vacancy number and interstitial number, gives positive values in the near surface region (which means vacancy is rich) and negative values in the deep depth (which means interstitial is rich). Note that Fe implants, the extra Fe atoms introduced, are treated as interstitials in the calculation. Due to defect sink property of a free surface, the surface region up to about 200 nm depth becomes void-depleted. Therefore, it is expected that void swelling will be

peaked at shallow depths, which is about half of the projected range of Fe, as observed by experiments.

The defect imbalance creates a serious problem for ion irradiation. If voids are enriched and promoted, it means true void swelling in reactors should be less, due to the fact that in reactor irradiation there is no such defect imbalance. In order to completely solve the problem, ion irradiation of multiple energies might be needed such that defect imbalance of each ion energy can be wiped out by other energies. Technologically, this can be achieved by using a rotating wheel to slow down beams. Ultra-thin metal films can be deposited on different regions of the wheel. Adjusting Al film thickness can change the beam energy after the beam penetration through the films.

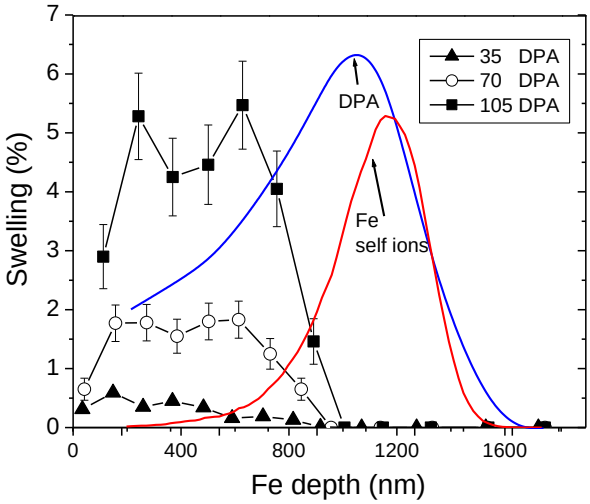


Fig. 1 Experimental void swelling distributions in pure Fe caused by 3.5 MeV Fe self ion irradiation at 450 ℃ for peak dpa values of 35, 70, and 105, respectively. The red curve is modeling obtained Fe implant distribution and the blue curve is modeling obtained dpa profile.

### 2.3 Rastering vs. defocusing

Many previous ion irradiation experiments were performed by using a rastering beam, which is ideal to achieve a good uniformity and also to irradiate multiple samples at the same time. For a specific position on a sample, its damage is equivalent to that from a pulsed beam, with pulse distance (time period of beam off) determined by beam scanning frequency. One serious issue of using rastering beam is that pulsed beam, in general, will suppress void swelling. Figure 2 is a comparison of void swelling in 3.5 MeV Fe-self-ion-irradiated Fe by using different beam scanning frequencies. Both void sizes and void densities are dramatically different at different scanning frequencies. Therefore, only defocusing beam should be used, since in reactors there is no such pulsing effect. A defocusing beam means that there is no scanning and beam is static on the sample [14].

The mechanism of void suppression under pulsed beam is complicated [15]. For metals, interstitials typically diffuse faster than vacancies. Therefore, pre-existing voids will first shrink upon interstitial absorption when a pulsed beam is on. Voids may grow again once vacancies begin to interact with them later. At longer time, voids will shrink again due to thermal emission of vacancies. It was argued by Ghoniem and Kulcinsk that if another interstitial pulse is introduced in the void shrinking stage, voids may eventually diminish once their sizes become less than the critical radius for growth [15].

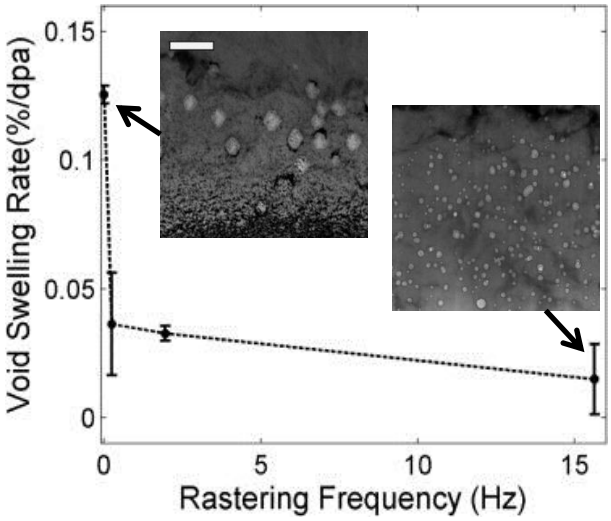


Fig.2 Experimental void swelling in pure Fe caused by 3.5 MeV Fe self ion irradiation at 450 ℃ for 150 peak dpa, as a function of beam scanning frequency. The frequency zero corresponds to a defocusing beam. The length scale is 250 nm for both cross sectional view of transmission electron microscopy images.

### 2.4 Multiple beam irradiation

Using a single beam for irradiation cannot include effects from transmutation gas atoms. Helium is the most important gas atoms to be considered due to its creation from neutron interactions with Ni, one major composition element in stainless steels. As a noble gas atom, helium has low solid solubility in metals and

they easily migrate and interact with vacancies or open volume defects. One major impact from helium is that voids easily form and are quickly stabilized. Helium-decorated vacancy expects to have higher energy barrier for interstitial-vacancy recombination. Helium-decorated voids expect to have smaller critical radius for void growth, due to pressure effects from helium inside voids. Therefore, voids prefer to grow and become stabilized at early stage of defect clustering.

Many ion accelerator laboratories in US have installed multiple ion beams to allow self-ion irradiation from one accelerator and helium ion irradiation from another accelerator simultaneously [16]. The ratios of helium to dpa need to be calculated for specific neutron spectra and target compositions.

However, although in general helium addition will increase void swelling, some recent data suggest that the effect of dual beam irradiation can be the opposite. Instead of creating more voids, higher ppm/dpa ratios can lead to suppressed void swelling, as shown by recent studies [17]. The detail mechanism is unclear.

### 2.5 Beam heating

Substrate temperatures for void swelling typically range from 300℃ to 600℃. The most important temperature is about 450℃, the peak swelling temperature for most Fe based steels [1]. Upon beam irradiation, locally deposited energy will add additional heating. Therefore, a heat stage requires temperature reading and auto adjustment of its power to maintain a designed temperature. There are a few potential problems: one is how samples are attached to the heat stage. If heat conductivity across sample-heater interface is not good enough, a temperature difference will appear. This is particular important for small specimen irradiation in which thermocouples for temperature measurements are attached to heater surface, instead of sample surface. Another problem is the temperature gradient caused by beam heating. If the specimen thickness is large, the temperature reading from the backside of the specimen will be much lower than the front surface being directly irradiated. To alleviate this issue, it is suggested that the metallic specimen thickness should be less than 1mm.

### 2.6 Beam monitoring

For room temperature irradiation, the beam current on a target can be easily measured by directly reading the current. Due to secondary electron ejection from a specimen surface, the target should be biased by adding a positive voltage, thus secondary electrons can return back to the surface to neutralize its charge. For high temperature irradiation, however, such direct current measurement is unrealistic due to thermal electron emission and also the complexity caused by heating stage setup. Typically, a Faraday cup is used to measure beam currents and is positioned well before the heat stage. The reading is regularly performed to get time averaged number for dose calculation. In addition to beam current, beam shape needs to be carefully monitored since dramatic shape changes means non-uniformity. One easy way is to visually monitor either ionoluminescence or IR signals from materials such as silica or quartz. These materials can be positioned on and off, in front of the specimen for regular checking.

## 3 Issues in modeling

Modeling is critical for verification and validation. The major modeling approaches include, from short to long time/length scales, quantum mechanics based density function theory (DFT), molecular dynamics simulations (MD), Monte Carlo simulations (MC), Kinetic Monte Carlo simulations (KMC), rate theory, and phase field theory. Each of these modeling has its own advantage and disadvantage. Efforts have been made during the past decades to develop multi-scale modeling approach, in order to predict structural evolutions linkable to experimental observations.

### 3.1 Monte Carlo simulations

In MC modeling, targets are often treated as random solids such that there is no need to memorize lattice locations of atoms. Simulations consider only binary collision—only one pair of projectile-target system is calculated for each collision. Neighboring atoms around a target atom are ignored in scattering calculations but some effects from neighboring atoms are considered by threshold displacement energy, which determines whether the scattered target atom will remain as a lattice atom with gained kinetic energy released as phonons or displaced by overcoming energy barrier required to break bonds. Even under such simplified treatment, computation is

still costly if each scattering follows standard mathematic treatments. Thanks for so called Magic Equation proposed by Biersack, computation time is greatly reduced and integration is replaced by an analytical expression [18]. Furthermore, the development of so called ZBL potentials (Ziegler-Biersack-Littmark) greatly reduces the computation complexity for specific ion-target system [19]. ZBL potential is a universial fitting which introduces reduced parameters to describe quantum mechanics predicted interatomic interactions as a function of ion-target separation distances. Nuclear stopping and electronic stopping are separated in modeling. Energy loss due to electronic stopping is considered only when atoms fly between two primary knock on events, while energy loss due to nuclear stopping is considered only when ion-target scattering occurs [18]. Computation speed is further increased by introducing so called free flying distances which ignore the scattering of small momentum transfer [18]. All these features are included in the Stopping and Range of Ions in Matter (SRIM, previously called TRIM) code [19]. For decades, SRIM code has been widely used to determine the ion fluence in experiments.

MC simulations have disadvantages that dynamic defect recombination cannot be simulated. Some previous studies use internationally increased threshold displacement energies to consider interstitials which are displaced far away from its original lattice sites and ignore those interstitial-vacancy pairs of close proximity [20]. But this approach is oversimplified to reveal details of defect annealing. Furthermore, defect interactions under complicated boundary conditions, such as interfaces and surfaces, cannot be simulated. MC simulations cannot consider effects of pre-existing features such as voids or phase segregation on defect creation.

### 3.2 Molecular dynamics simulations

MD simulations consider the effects from all atoms in a cell, which typically have millions of atoms or more. The structural evolutions are modeled by considering all interatomic interactions, with position change of each individual atom determined by forces from the rest of the cell atoms [21]. Nevertheless, its computation cost is high.

MD simulations are very powerful to reveal details of damage cascade evolution which include (1) collision stage in which high density defects are created along an ion track; (2) thermal spike stage in which kinetic energies of all displaced atoms convert to phonon and energy sharing between neighboring atoms may lead to temporary melting in a cascade core; (3) defect annealing stage in which heat dissipates from the cascade core and high density defects have dynamic interactions, and stable defects form.

MD simulations are ideal to reveal defect-boundary interactions and shed light onto fundamentals. This is particularly important for structures of high surface to volume ratios such as nanolayers or nano-grained engineered materials. For example, Figure 3 compares radiation damage in pure Fe with (a-1 to a-3) or without (b-1 to b-3) a grain boundary. Due to defect sink properties of a grain boundary, defects in close proximity of the boundary migrate towards, get trapped and annihilate on the boundary. Such defect-boundary interactions cannot be simply explained by defect formation energy difference in the bulk and on a grain boundary. Traditional theory explains the defect trapping as biased random diffusions towards a boundary. Recent modeling studies, however, suggest that defect-boundary interaction mechanism is much more complicated. Both defect loading and annihilation at a grain boundary involves correlated movements of a group of atoms, by forming so called chain-like defects [6].

MD simulation, however, has its own limits. First of all, MD simulations do not consider electron subsystems. Any collision process which disturbs electrons cannot be modeled. One for example, for swift ion irradiation which has extremely high electronic stopping power, electron excitation and subsequent electron-phonon coupling can create substantial temperature rises high enough for local melting. The collision may also lead to partial or complete ionization of target atoms along the ion track, creating a zone in which strong Coulomb repulsive forces among positively charged atoms lead to so called Coulomb explosion [22]. These details are difficult to model by using MD simulation directly, unless the simulation is coupled with other methods to estimate the temperature changes from electron heating and electron-phonon interactions in the

thermal spike model or to introduce an ionization function in the Coulomb explosion model.

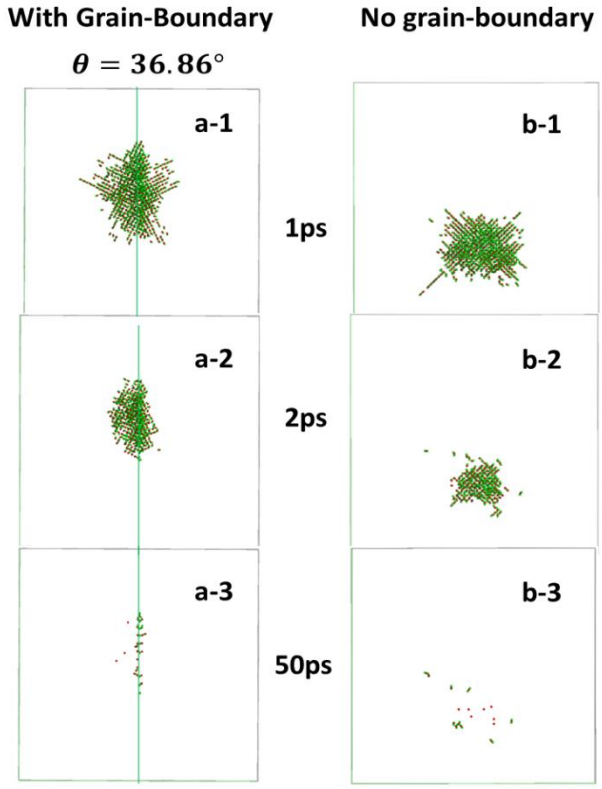


Fig. 3 MD simulations of damage cascade developments caused by 2 keV Fe atom in Fe (a) containing a grain boundary and (b) without a grain boundary.

Although accelerated MD simulations have been utilized to speed up modeling, by either intentionally increasing the cell temperature or reducing energy barrier heights for defect reactions, both time and length scales still represent great limits. Usually the cell size cannot be larger than one micron and the time cannot be longer than 1 ns. Since defect clustering observed from experiments corresponds to time scales of seconds to years, MD method is not realistic to predict structural evolution comparable to lab observations.

### 3.3 Kinetic Monte Carlo simulations

KMC simulations are often used as a method to overcome limits from MD simulations for longer time scale and larger length scale [23]. In KMC approach, all possible defect reactions are considered and a random number is generated to select one particular defect reaction. The selection is randomly determined, but, after many trials the reaction selections will statistically follow the probabilities determined by energy barriers of these reactions.

As one example, Fig. 4 shows defect reactions in Fe irradiated by 1 MeV Fe self ions. The positions of interstitials and vacancies, created from 100 damage cascades, are obtained from Monte Carlo simulations and are used as inputs for KMC simulations. Majority of defects are annihilated but a small fraction of them survive and form defect clusters. Vacancy clusters are immobile but interstitial dislocation loops are highly mobile. At longest annealing time, large voids are clearly observable, which agree with experimental observations.

KMC method, however, requires kinetics information for all allowable defect reactions. The modeling cannot predict new reaction path. Instead, all defect reactions and associated energy barriers must be known first. These kinetics often require MD simulations to obtain externally. Since defect clustering process may involve defect sizes up to a few thousands of atoms and beyond, it is difficult to obtain all kinetics. Certain empirical fitting or approximations are often needed.

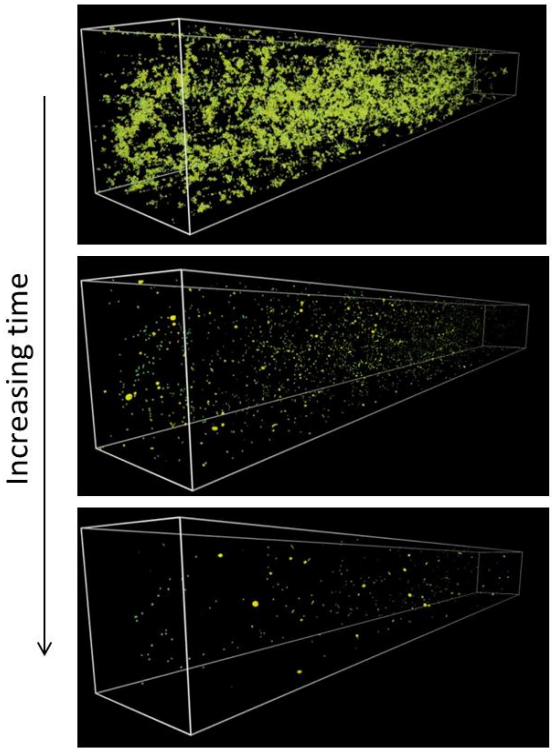


Fig. 4 KMC simulations of defect clustering in Fe caused by 1 MeV Fe ions, with increasing time. The yellow refers to interstitials and green refers to vacancies.

### 3.4 Rate theory

Rate theory calculates spatial and temporal distribution of specific defect types by solving coupled diffusion equation [24]. Each defect type, *i.e.* defects of particular cluster size, is represented by one equation which considers diffusion, creation and annihilation. Due to defect interactions, these equations are coupled with each other and need to be solved simultaneously.

Similar to KMC method, rate theory can predict defect size and density changes upon annealing but it cannot predict new defect reaction paths. The largest limitation of rate theory calculation is that all defect kinetics must be known first, which require MD simulation or other methods to obtain externally.

In a typical reaction equation to describe one defect cluster, it includes the gain term in which smaller defect cluster traps point defects to grow into this particular size, and loss term in which point defects are thermally emitted. Such growth and decay reveals fundamentals of defect clustering process: although defect clusters such as voids are not mobile, they can interact with each other through exchanging point defects. Interactions of point defects with defect clusters can quickly reach static steady states in which the population of point defects (locally around the defect clusters) is determined by the binding energy of defect clusters. The higher the binding energy, the high the energy barrier for thermal emission/dissociation, and the less the point defect surrounding the defect cluster. For a system including defect clusters of different sizes, binding energies of larger defect clusters typically increase with increasing sizes. Therefore, point defect surrounding small defect clusters will diffuse toward the region surrounding large defect clusters, driven by a concentration gradient. This is the reason why defects become larger and larger upon thermal annealing.

In previous studies by Cowern *et al.* [24], the averaged point defect concentrations as a function of annealing time are experimentally detected. Then rate theory is used to match the data, by adjusting the binding energies of defect clusters. This unique method is able to extract formation energies of all defect clusters, as a function of their sizes. Defect interactions such as damage cascade annealing start at a time scale (<1ps) which is beyond experimental detection limits. Defect kinetics of small defect clusters, however, sensitively determines the subsequent growth to large defect clusters. For example, any small defect clusters having low formation energy will slow down the size evolution towards large defect clusters. Therefore, information obtained at longer time scales, which are comparable to experiments, can reveal details at early defect clustering stage which cannot be measured directly. Cowern's approach might be one realistic solution to meet the needs from both rate theory or KMC simulations.

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